

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptaul29pxo

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	JAN 11	CA/CAPLUS - Expanded patent coverage to include Russia (Federal Institute of Industrial Property)
NEWS EXPRESS			JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information
NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:23:39 ON 24 JAN 2005

=>

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

8.19

8.19

FILE 'REGISTRY' ENTERED AT 09:46:46 ON 24 JAN 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JAN 2005 HIGHEST RN 819046-01-0

DICTIONARY FILE UPDATES: 23 JAN 2005 HIGHEST RN 819046-01-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\STNEXP4\QUERIES\aw1.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\STNEXP4\QUERIES\aw2.str

L2 STRUCTURE UPLOADED

=>

Uploading C:\STNEXP4\QUERIES\aw3.str

L3 STRUCTURE UPLOADED

=> s 11
SAMPLE SEARCH INITIATED 09:50:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 61448 TO ITERATE

1.6% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 0

L4 0 SEA SSS SAM L1

=>
=>

Uploading C:\STNEXP4\QUERIES\aw4.str

L5 STRUCTURE UPLOADED

=> s 15
SAMPLE SEARCH INITIATED 10:09:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 34843 TO ITERATE

2.9% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 685710 TO 708010
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=>

Uploading C:\STNEXP4\QUERIES\aw5.str

L7 STRUCTURE UPLOADED

=> s 17
SAMPLE SEARCH INITIATED 10:13:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 49340 TO ITERATE

2.0% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 973556 TO 1000044
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=>

Uploading C:\STNEXP4\QUERIES\aw6.str

L9 STRUCTURE UPLOADED

=> s 19

SAMPLE SEARCH INITIATED 10:18:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 46756 TO ITERATE

2.1% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 922223 TO 948017
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

=>

=>

Uploading C:\STNEXP4\QUERIES\aw7.str

L11 STRUCTURE UPLOADED

=> s 111

SAMPLE SEARCH INITIATED 10:20:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4837 TO ITERATE

20.7% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 92570 TO 100910
PROJECTED ANSWERS: 0 TO 0

L12 0 SEA SSS SAM L11

=>

Uploading C:\STNEXP4\QUERIES\aw8.str

L13 STRUCTURE UPLOADED

=> s 113

SAMPLE SEARCH INITIATED 10:21:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 10214 TO ITERATE

9.8% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 198224 TO 210336
PROJECTED ANSWERS: 0 TO 0

L14 0 SEA SSS SAM L13

```

=> search l11
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:21:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 96489 TO ITERATE

100.0% PROCESSED 96489 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.14

L15 0 SEA SSS FUL L11

=> search l13
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:22:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 203759 TO ITERATE

100.0% PROCESSED 203759 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.13

L16 0 SEA SSS FUL L13

=>
Uploading C:\STNEXP4\QUERIES\awl0.str

L17 STRUCTURE UPLOADED

=>
Uploading C:\STNEXP4\QUERIES\aw9.str

L18 STRUCTURE UPLOADED

=> s l17
SAMPLE SEARCH INITIATED 10:25:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4837 TO ITERATE

20.7% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED ITERATIONS: 92570 TO 100910
PROJECTED ANSWERS: 0 TO 0

L19 0 SEA SSS SAM L17

=> search l17
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:25:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 96489 TO ITERATE

100.0% PROCESSED 96489 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.15

L20 0 SEA SSS FUL L17

```

=> s 118
SAMPLE SEARCH INITIATED 10:26:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 10214 TO ITERATE

9.8% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 198224 TO 210336
PROJECTED ANSWERS: 0 TO 0

L21 0 SEA SSS SAM L18

=> search 118
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:26:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 203759 TO ITERATE

100.0% PROCESSED 203759 ITERATIONS
SEARCH TIME: 00.00.14

21 ANSWERS

L22 21 SEA SSS FUL L18

=>
Uploading C:\STNEXP4\QUERIES\all.str

L23 STRUCTURE UPLOADED

=> d 123
L23 HAS NO ANSWERS
L23 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 123
SAMPLE SEARCH INITIATED 10:32:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 177 TO ITERATE

100.0% PROCESSED 177 ITERATIONS (19 INCOMPLETE)
SEARCH TIME: 00.00.03

19 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2742 TO 4338
PROJECTED ANSWERS: 119 TO 641

L24 19 SEA SSS SAM L23

=> s 123
SAMPLE SEARCH INITIATED 10:32:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 177 TO ITERATE

100.0% PROCESSED 177 ITERATIONS (19 INCOMPLETE)

19 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2742 TO 4338
PROJECTED ANSWERS: 119 TO 641

L25 19 SEA SSS SAM L23

=> search l23

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:33:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3334 TO ITERATE

100.0% PROCESSED 3334 ITERATIONS (300 INCOMPLETE) 300 ANSWERS
SEARCH TIME: 00.00.11

L26 300 SEA SSS FUL L23

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	838.04	846.23

FILE 'CAPLUS' ENTERED AT 10:33:22 ON 24 JAN 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 24 Jan 2005 VOL 142 ISS 5
FILE LAST UPDATED: 23 Jan 2005 (20050123/ED)

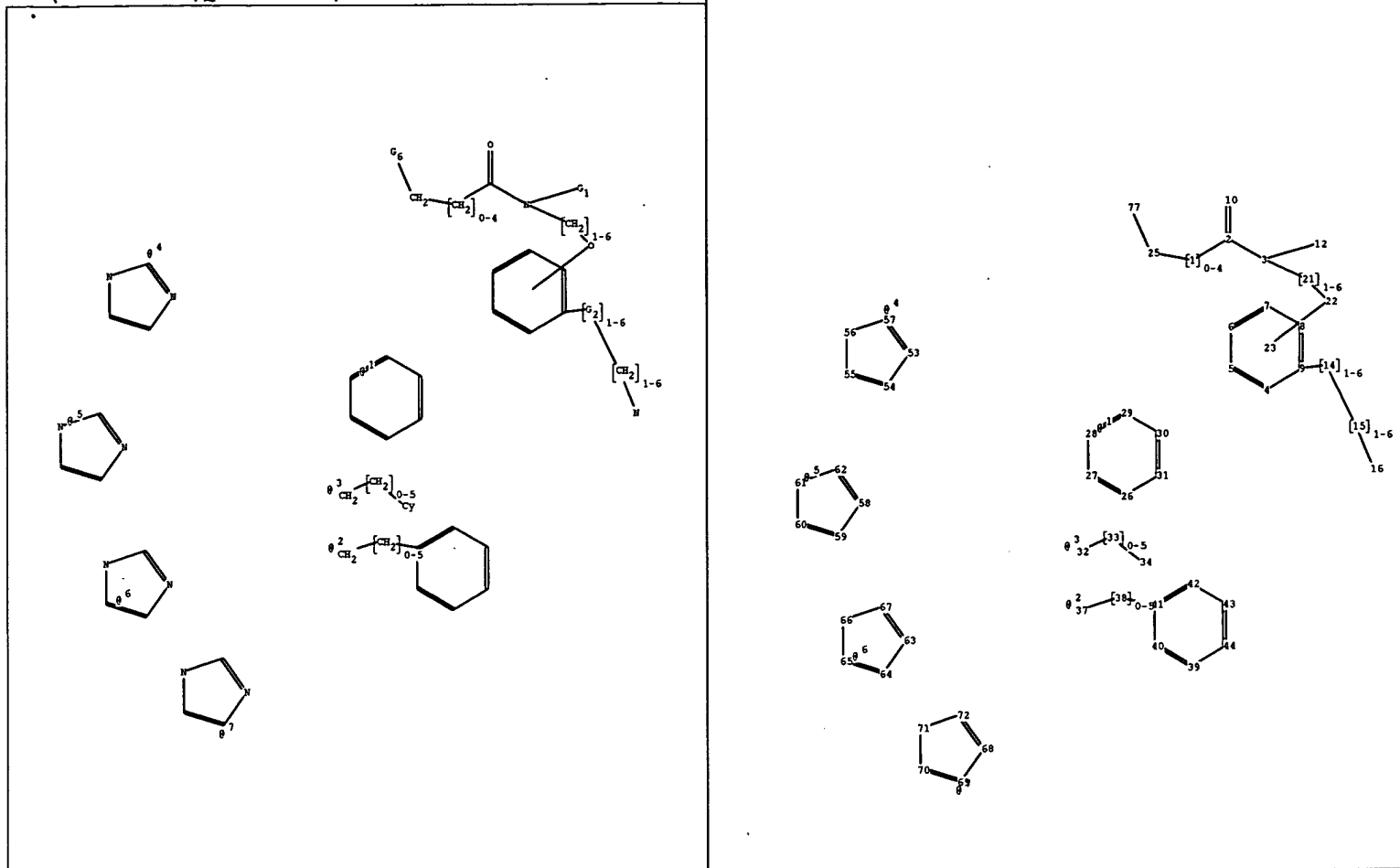
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l26

L27 123 L26

=> d l27 fbib ab hitstr 1-123

L27 ANSWER 1 OF 123 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:1059377 CAPLUS
DN 142:19573
TI Purification means
IN Hay, Alastair; Cotton, Graham; Ramage, Robert
PA CSS-Albachem Limited, UK



chain nodes :

1 2 3 10 12 14 15 16 21 22 25 32 33 34 37 38 77

ring nodes :

4 5 6 7 8 9 26 27 28 29 30 31 39 40 41 42 43 44 53 54
55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72

chain bonds :

1-2 1-25 2-3 2-10 3-12 3-21 9-14 14-15 15-16 21-22 25-77 32-33
33-34 37-38 38-41

ring bonds :

4-5 4-9 5-6 6-7 7-8 8-9 26-27 26-31 27-28 28-29 29-30 30-31
39-40 39-44 40-41 41-42 42-43 43-44 53-54 53-57 54-55 55-56
56-57 58-59 58-62 59-60 60-61 61-62 63-64 63-67 64-65 65-66
66-67 68-69 68-72 69-70 70-71 71-72

exact/norm bonds :

2-3 2-10 3-12 9-14 14-15 25-77 33-34 53-54 53-57 54-55 55-56
56-57 58-59 58-62 59-60 60-61 61-62 63-64 63-67 64-65 65-66
66-67 68-69 68-72 69-70 70-71 71-72

exact bonds :

1-2 1-25 3-21 15-16 21-22 32-33 37-38 38-41

normalized bonds :

4-5 4-9 5-6 6-7 7-8 8-9 26-27 26-31 27-28 28-29 29-30 30-31
39-40 39-44 40-41 41-42 42-43 43-44

G1:H,Ak

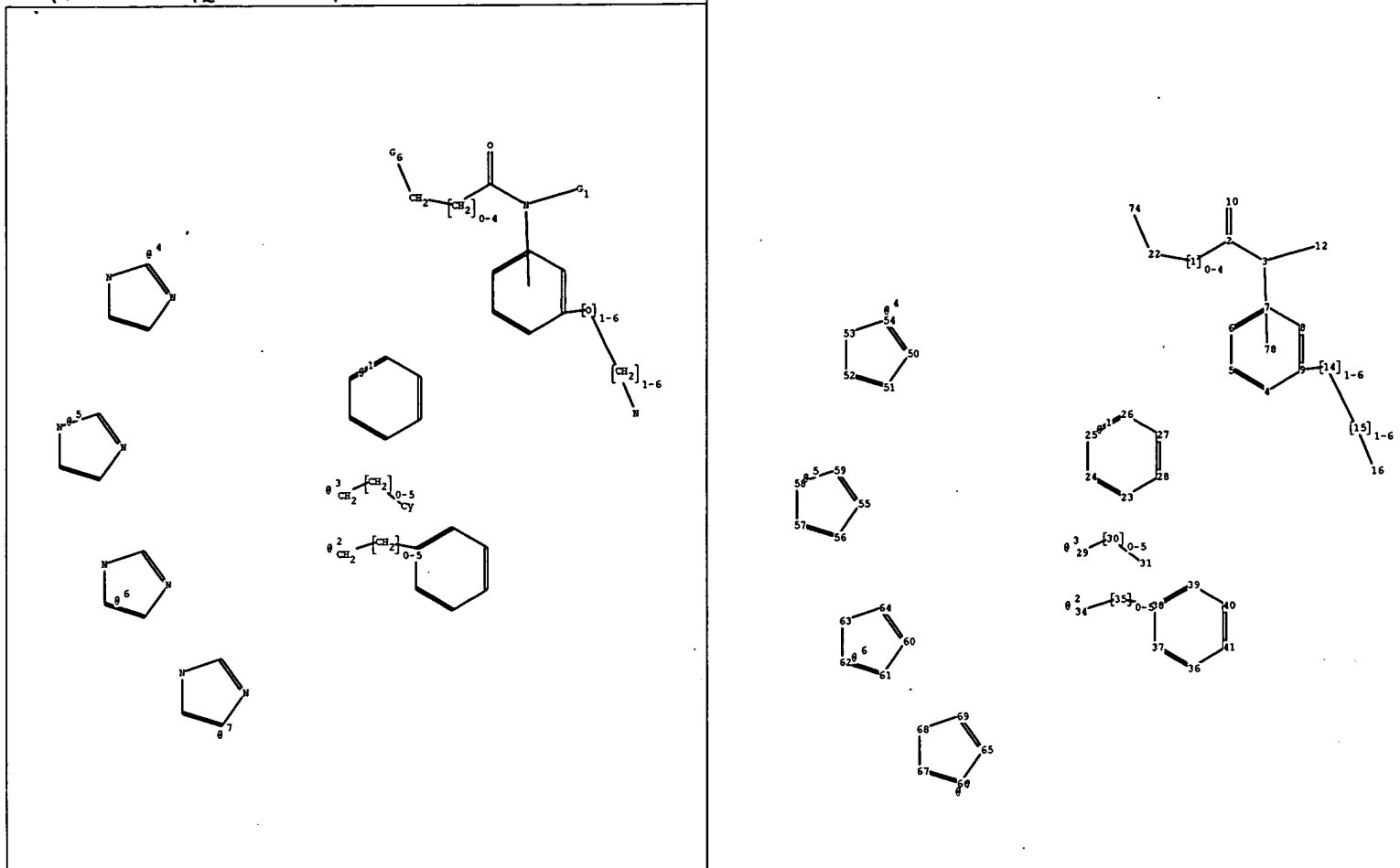
G2:O,N,C

G3:O,CH2


```

1:CLASS 2:CLASS 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 21:CLASS 22:CLASS
23:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:CLASS 33:CLASS 34:Atom 37:CLASS 38:CLASS 39:Atom 40:Atom
41:Atom 42:Atom 43:Atom 44:Atom 53:Atom 54:Atom 55:Atom 56:Atom
57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom
65:Atom 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom
77:CLASS

```



chain nodes :

1 2 3 10 12 14 15 16 22 29 30 31 34 35 74

ring nodes :

4 5 6 7 8 9 23 24 25 26 27 28 36 37 38 39 40 41 50 51
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69

chain bonds :

1-2 1-22 2-3 2-10 3-12 9-14 14-15 15-16 22-74 29-30 30-31
34-35 35-38

ring bonds :

4-5 4-9 5-6 6-7 7-8 8-9 23-24 23-28 24-25 25-26 26-27 27-28
36-37 36-41 37-38 38-39 39-40 40-41 50-51 50-54 51-52 52-53
53-54 55-56 55-59 56-57 57-58 58-59 60-61 60-64 61-62 62-63
63-64 65-66 65-69 66-67 67-68 68-69

exact/norm bonds :

2-3 2-10 3-12 9-14 22-74 30-31 50-51 50-54 51-52 52-53 53-54
55-56 55-59 56-57 57-58 58-59 60-61 60-64 61-62 62-63 63-64
65-66 65-69 66-67 67-68 68-69

exact bonds :

1-2 1-22 14-15 15-16 29-30 34-35 35-38

normalized bonds :

4-5 4-9 5-6 6-7 7-8 8-9 23-24 23-28 24-25 25-26 26-27 27-28
36-37 36-41 37-38 38-39 39-40 40-41

G1:H,Ak

G2:O,N,C

G3:O,CH2

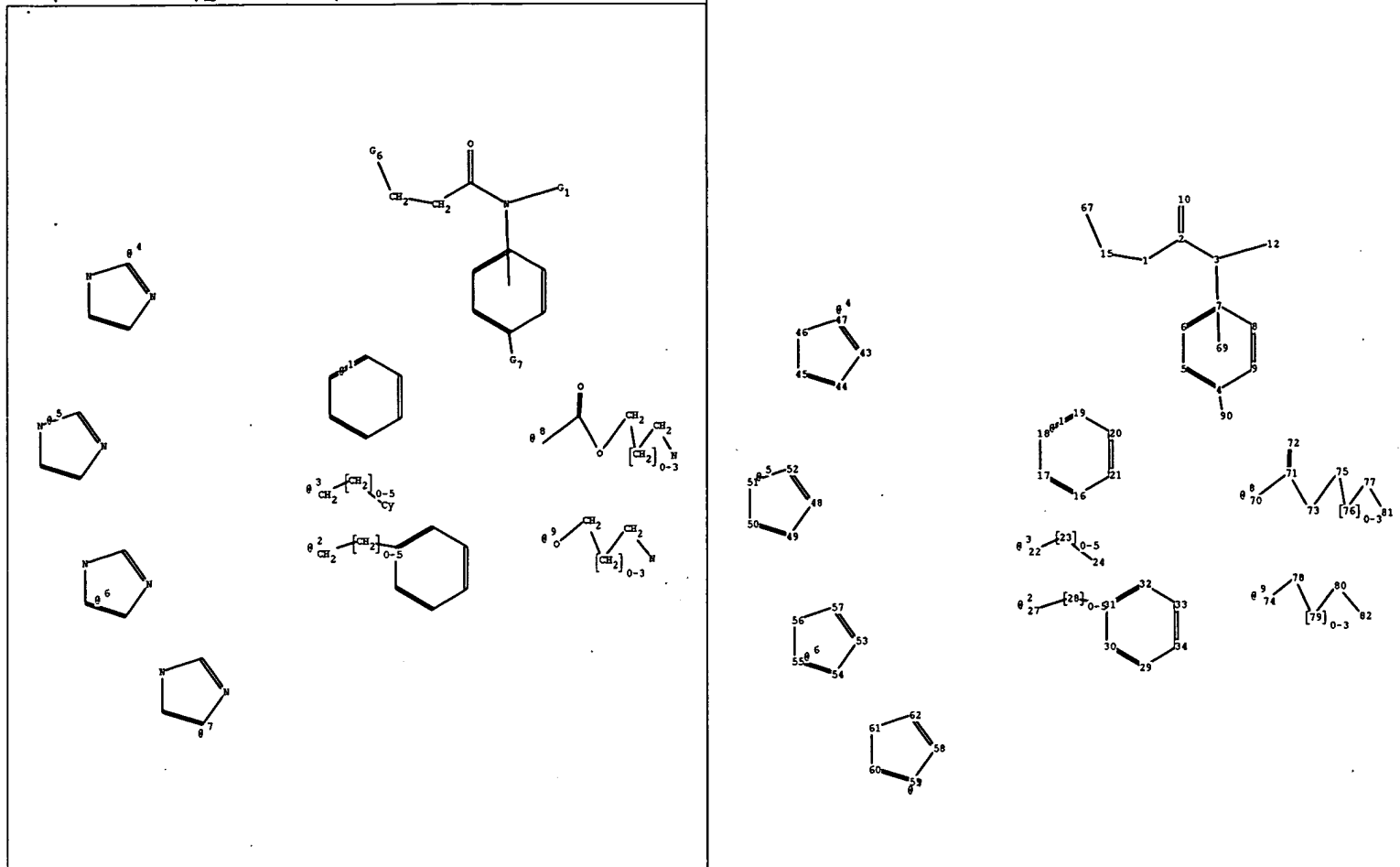
G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

Match level :

1:CLASS	2:CLASS	3:CLASS	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom
10:CLASS	12:CLASS	14:CLASS	15:CLASS	16:CLASS	22:CLASS	23:Atom		
24:Atom	25:Atom	26:Atom	27:Atom	28:Atom	29:CLASS	30:CLASS	31:Atom	
34:CLASS	35:CLASS	36:Atom	37:Atom	38:Atom	39:Atom	40:Atom	41:Atom	
50:Atom	51:Atom	52:Atom	53:Atom	54:Atom	55:Atom	56:Atom	57:Atom	
58:Atom	59:Atom	60:Atom	61:Atom	62:Atom	63:Atom	64:Atom	65:Atom	
66:Atom	67:Atom	68:Atom	69:Atom	74:CLASS	78:CLASS			



chain nodes :

1 2 3 10 12 15 22 23 24 27 28 67 70 71 72 73 74 75 76
77 78 79 80 81 82 90

ring nodes :

4 5 6 7 8 9 16 17 18 19 20 21 29 30 31 32 33 34 43 44
45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62

chain bonds :

1-2 1-15 2-3 2-10 3-12 4-90 15-67 22-23 23-24 27-28 28-31
70-71 71-72 71-73 73-75 74-78 75-76 76-77 77-81 78-79 79-80
80-82

ring bonds :

4-5 4-9 5-6 6-7 7-8 8-9 16-17 16-21 17-18 18-19 19-20 20-21
29-30 29-34 30-31 31-32 32-33 33-34 43-44 43-47 44-45 45-46
46-47 48-49 48-52 49-50 50-51 51-52 53-54 53-57 54-55 55-56
56-57 58-59 58-62 59-60 60-61 61-62

exact/norm bonds :

2-3 2-10 3-12 4-90 15-67 23-24 43-44 43-47 44-45 45-46 46-47
48-49 48-52 49-50 50-51 51-52 53-54 53-57 54-55 55-56 56-57
58-59 58-62 59-60 60-61 61-62 71-72 71-73

exact bonds :

1-2 1-15 22-23 27-28 28-31 70-71 73-75 74-78 75-76 76-77 77-81
78-79 79-80 80-82

normalized bonds :

4-5 4-9 5-6 6-7 7-8 8-9 16-17 16-21 17-18 18-19 19-20 20-21
29-30 29-34 30-31 31-32 32-33 33-34

G2:O,N,C

G3:O,CH2

G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

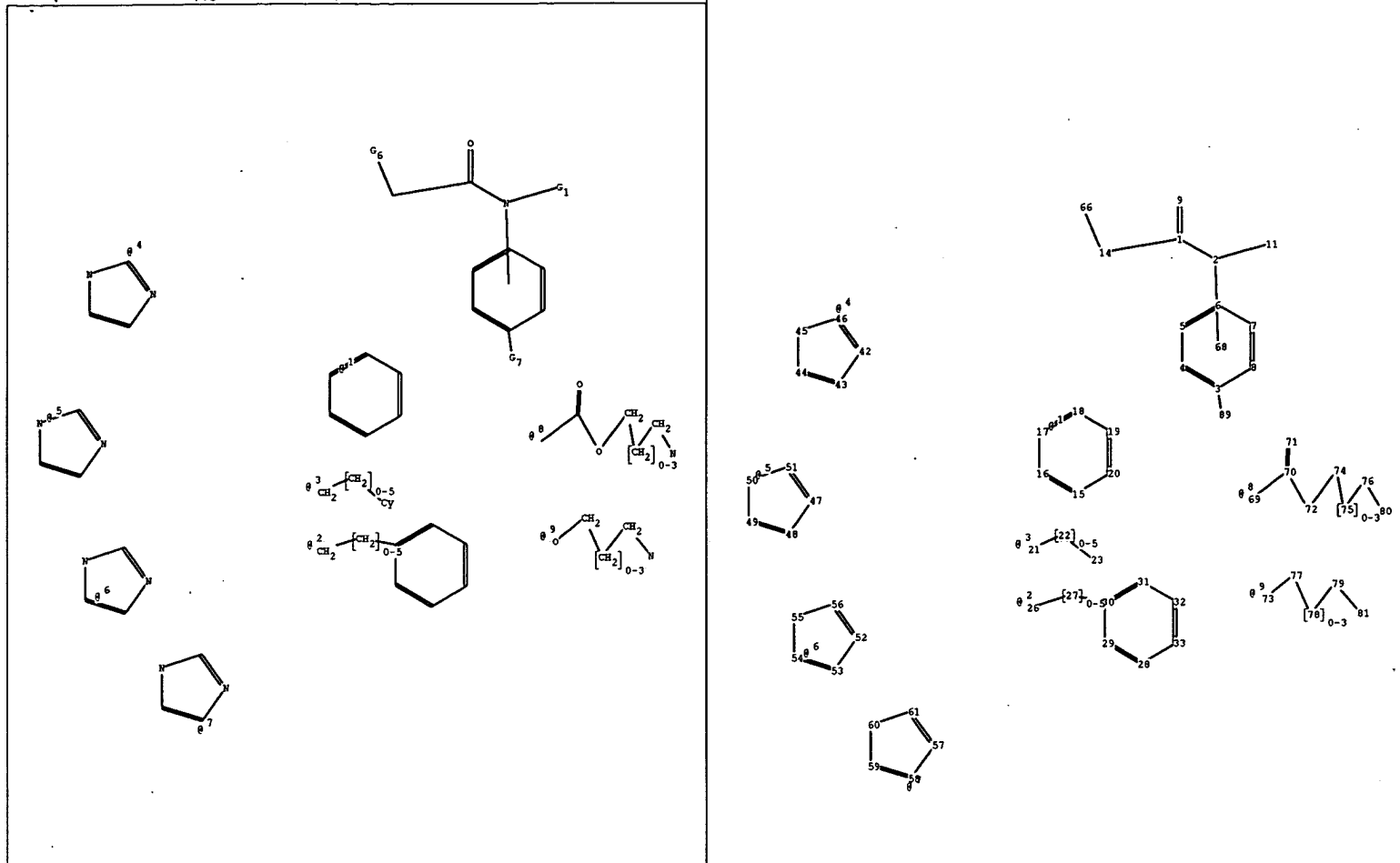
G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

G7:[*8],[*9]

Match level :

1:CLASS	2:CLASS	3:CLASS	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom
10:CLASS	12:CLASS	15:CLASS	16:Atom	17:Atom	18:Atom	19:Atom	20:Atom	
21:Atom	22:CLASS	23:CLASS	24:Atom	27:CLASS	28:CLASS	29:Atom		
30:Atom	31:Atom	32:Atom	33:Atom	34:Atom	43:Atom	44:Atom	45:Atom	
46:Atom	47:Atom	48:Atom	49:Atom	50:Atom	51:Atom	52:Atom	53:Atom	
54:Atom	55:Atom	56:Atom	57:Atom	58:Atom	59:Atom	60:Atom	61:Atom	
62:Atom	67:CLASS	69:CLASS	70:CLASS	71:CLASS	72:CLASS	73:CLASS		
74:CLASS	75:CLASS	76:CLASS	77:CLASS	78:CLASS	79:CLASS	80:CLASS		
81:CLASS	82:CLASS	90:CLASS						



chain nodes :

1 2 9 11 14 21 22 23 26 27 66 69 70 71 72 73 74 75 76
77 78 79 80 81 89

ring nodes :

3 4 5 6 7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 43
44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61

chain bonds :

1-9 1-2 1-14 2-11 3-89 14-66 21-22 22-23 26-27 27-30 69-70
70-71 70-72 72-74 73-77 74-75 75-76 76-80 77-78 78-79 79-81

ring bonds :

3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45 44-45
45-46 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55
55-56 57-58 57-61 58-59 59-60 60-61

exact/norm bonds :

1-9 1-2 2-11 3-89 14-66 22-23 42-43 42-46 43-44 44-45 45-46
47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55 55-56
57-58 57-61 58-59 59-60 60-61 70-71 70-72

exact bonds :

1-14 21-22 26-27 27-30 69-70 72-74 73-77 74-75 75-76 76-80
77-78 78-79 79-81

normalized bonds :

3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33

G1:H,Ak

G2:O,N,C

G3:O,CH2

G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

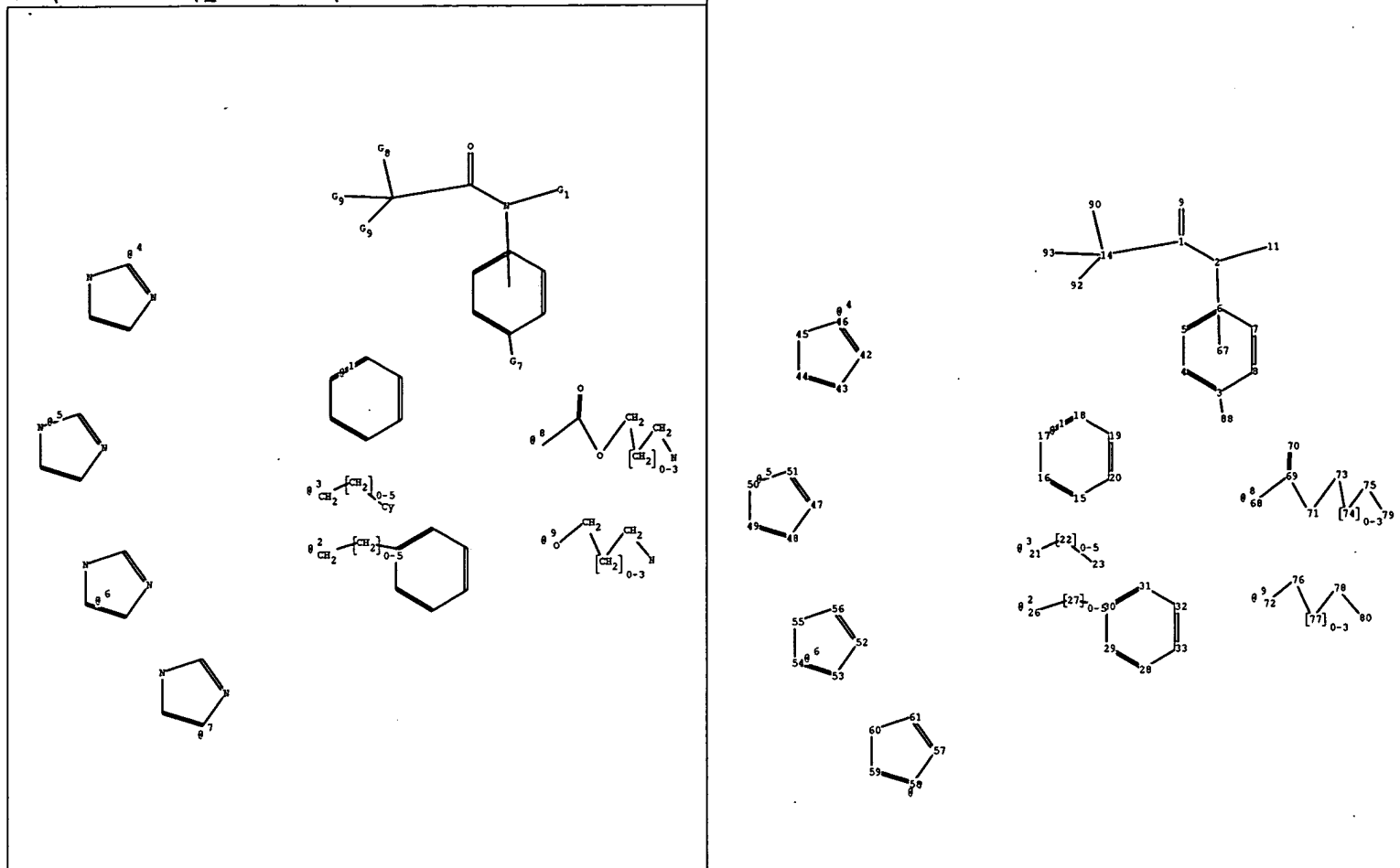
G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

G7:[*8],[*9]

Match level :

1:CLASS	2:CLASS	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:CLASS
11:CLASS	14:CLASS	15:Atom	16:Atom	17:Atom	18:Atom	19:Atom	20:Atom	
21:CLASS	22:CLASS	23:Atom	26:CLASS	27:CLASS	28:Atom	29:Atom		
30:Atom	31:Atom	32:Atom	33:Atom	42:Atom	43:Atom	44:Atom	45:Atom	
46:Atom	47:Atom	48:Atom	49:Atom	50:Atom	51:Atom	52:Atom	53:Atom	
54:Atom	55:Atom	56:Atom	57:Atom	58:Atom	59:Atom	60:Atom	61:Atom	
66:CLASS	68:CLASS	69:CLASS	70:CLASS	71:CLASS	72:CLASS	73:CLASS		
74:CLASS	75:CLASS	76:CLASS	77:CLASS	78:CLASS	79:CLASS	80:CLASS		
81:CLASS	89:CLASS							



chain nodes :

1 2 9 11 14 21 22 23 26 27 68 69 70 71 72 73 74 75 76
77 78 79 80 88 90 92 93

ring nodes :

3 4 5 6 7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 43
44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61

chain bonds :

1-9 1-2 1-14 2-11 3-88 14-90 14-92 14-93 21-22 22-23 26-27
27-30 68-69 69-70 69-71 71-73 72-76 73-74 74-75 75-79 76-77
77-78 78-80

ring bonds :

3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45
45-46 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55
55-56 57-58 57-61 58-59 59-60 60-61

exact/norm bonds :

1-9 1-2 2-11 3-88 14-90 14-92 14-93 22-23 42-43 42-46 43-44
44-45 45-46 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54
54-55 55-56 57-58 57-61 58-59 59-60 60-61 69-70 69-71

exact bonds :

1-14 21-22 26-27 27-30 68-69 71-73 72-76 73-74 74-75 75-79
76-77 77-78 78-80

normalized bonds :

3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33

G2:O,N,C

G3:O,CH2

G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

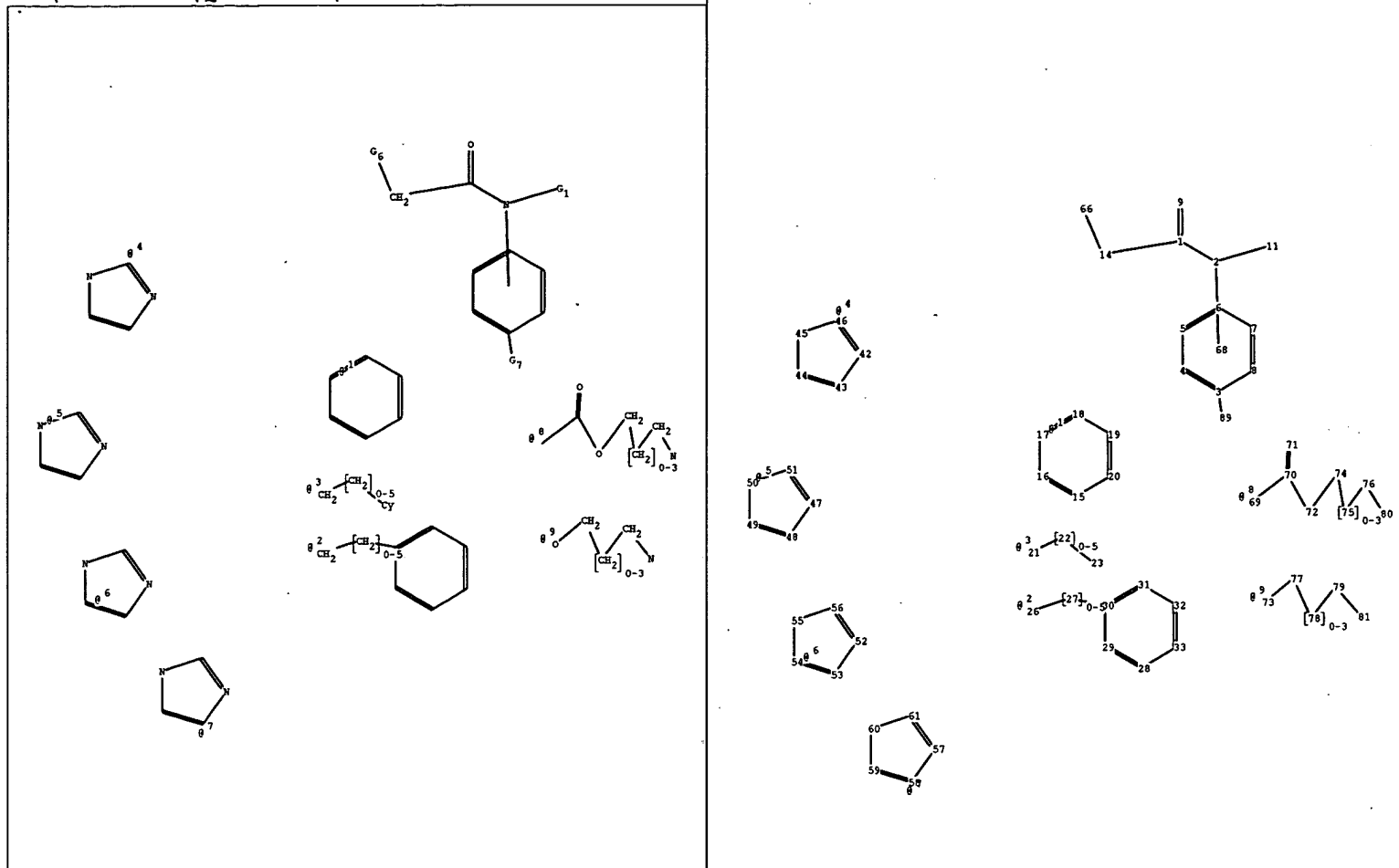
G7:[*8],[*9]

G8:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1]

G9:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1]

Match level :

1:CLASS	2:CLASS	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:CLASS
11:CLASS	14:CLASS	15:Atom	16:Atom	17:Atom	18:Atom	19:Atom	20:Atom	
21:CLASS	22:CLASS	23:Atom	26:CLASS	27:CLASS	28:Atom	29:Atom		
30:Atom	31:Atom	32:Atom	33:Atom	42:Atom	43:Atom	44:Atom	45:Atom	
46:Atom	47:Atom	48:Atom	49:Atom	50:Atom	51:Atom	52:Atom	53:Atom	
54:Atom	55:Atom	56:Atom	57:Atom	58:Atom	59:Atom	60:Atom	61:Atom	
67:CLASS	68:CLASS	69:CLASS	70:CLASS	71:CLASS	72:CLASS	73:CLASS		
74:CLASS	75:CLASS	76:CLASS	77:CLASS	78:CLASS	79:CLASS	80:CLASS		
88:CLASS	90:CLASS	92:CLASS	93:CLASS					



chain nodes :

1 2 9 11 14 21 22 23 26 27 66 69 70 71 72 73 74 75 76
77 78 79 80 81 89

ring nodes :

3 4 5 6 7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 43
44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61

chain bonds :

1-9 1-2 1-14 2-11 3-89 14-66 21-22 22-23 26-27 27-30 69-70
70-71 70-72 72-74 73-77 74-75 75-76 76-80 77-78 78-79 79-81

ring bonds :

3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45 44-45
45-46 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55
55-56 57-58 57-61 58-59 59-60 60-61

exact/norm bonds :

1-9 1-2 2-11 3-89 14-66 22-23 42-43 42-46 43-44 44-45 45-46
47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55 55-56
57-58 57-61 58-59 59-60 60-61 70-71 70-72

exact bonds :

1-14 21-22 26-27 27-30 69-70 72-74 73-77 74-75 75-76 76-80
77-78 78-79 79-81

normalized bonds :

3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33

G1:H, Ak

G2:O, N, C

G3:O,CH2

G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

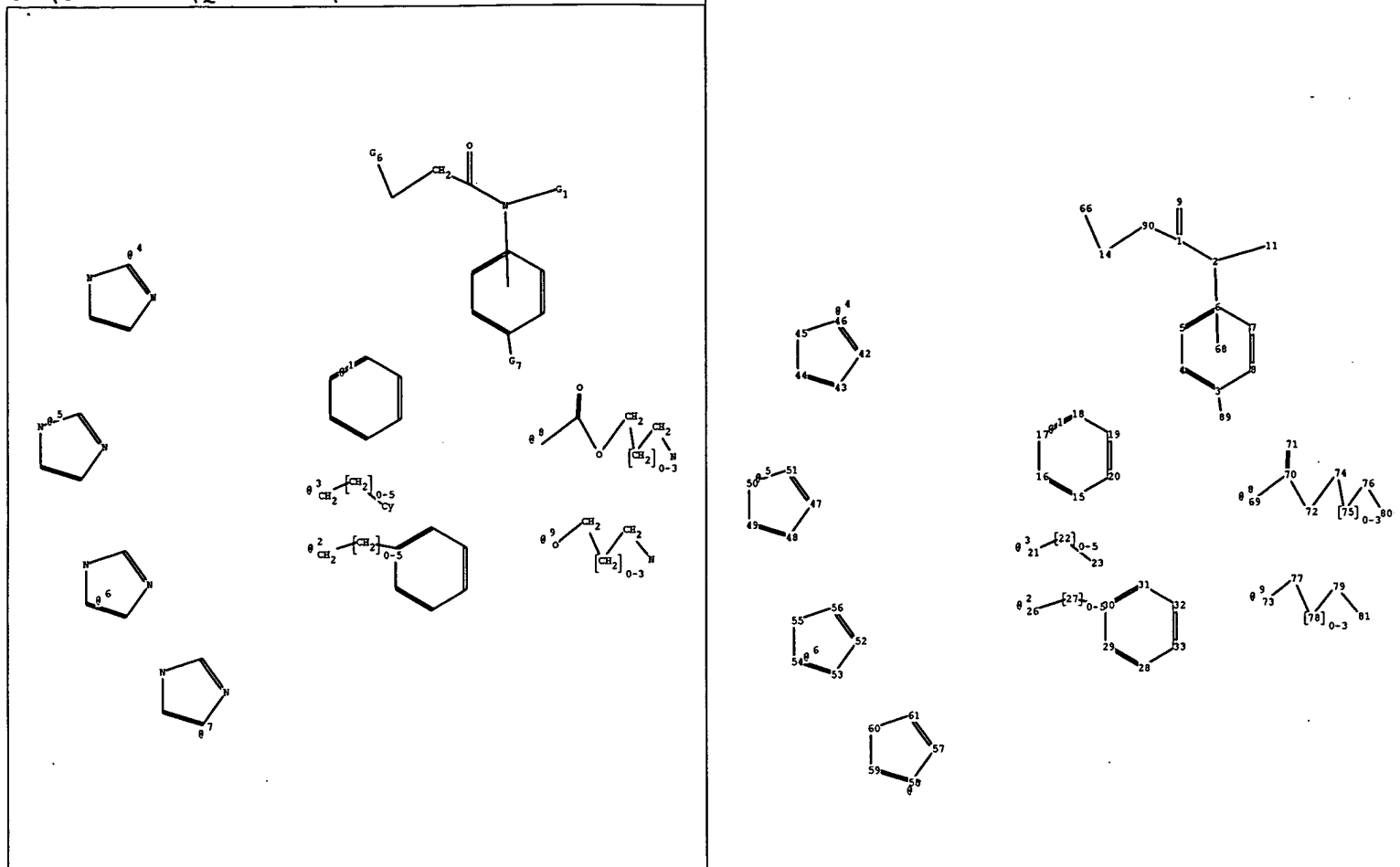
G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

G7:[*8],[*9]

Match level :

1:CLASS	2:CLASS	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:CLASS
11:CLASS	14:CLASS	15:Atom	16:Atom	17:Atom	18:Atom	19:Atom	20:Atom	
21:CLASS	22:CLASS	23:Atom	26:CLASS	27:CLASS	28:Atom	29:Atom		
30:Atom	31:Atom	32:Atom	33:Atom	42:Atom	43:Atom	44:Atom	45:Atom	
46:Atom	47:Atom	48:Atom	49:Atom	50:Atom	51:Atom	52:Atom	53:Atom	
54:Atom	55:Atom	56:Atom	57:Atom	58:Atom	59:Atom	60:Atom	61:Atom	
66:CLASS	68:CLASS	69:CLASS	70:CLASS	71:CLASS	72:CLASS	73:CLASS		
74:CLASS	75:CLASS	76:CLASS	77:CLASS	78:CLASS	79:CLASS	80:CLASS		
81:CLASS	89:CLASS							



chain nodes :

1 2 9 11 14 21 22 23 26 27 66 69 70 71 72 73 74 75 76
77 78 79 80 81 89 90

ring nodes :

3 4 5 6 7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 43
44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61

chain bonds :

1-9 1-2 1-90 2-11 3-89 14-66 14-90 21-22 22-23 26-27 27-30
69-70 70-71 70-72 72-74 73-77 74-75 75-76 76-80 77-78 78-79
79-81

ring bonds :

3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45 44-45
45-46 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55 55-56
55-56 57-58 57-61 58-59 59-60 60-61

exact/norm bonds :

1-9 1-2 2-11 3-89 14-66 22-23 42-43 42-46 43-44 44-45 45-46
47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55 55-56
57-58 57-61 58-59 59-60 60-61 70-71 70-72

exact bonds :

1-90 14-90 21-22 26-27 27-30 69-70 72-74 73-77 74-75 75-76
76-80 77-78 78-79 79-81

normalized bonds :

3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33

G2:O, N, C

G3:O, CH2

G4:H, CH3, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*1], [*2]

G5:CH3, Et, n-Pr, i-Pr, i-Bu, s-Bu, t-Bu, [*1], [*3]

G6:NH2, NH, [*1], [*4], [*5], [*6], [*7]

G7:[*8], [*9]

Match level :

1:CLASS	2:CLASS	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:CLASS
11:CLASS	14:CLASS	15:Atom	16:Atom	17:Atom	18:Atom	19:Atom	20:Atom	
21:CLASS	22:CLASS	23:Atom	26:CLASS	27:CLASS	28:Atom	29:Atom		
30:Atom	31:Atom	32:Atom	33:Atom	42:Atom	43:Atom	44:Atom	45:Atom	
46:Atom	47:Atom	48:Atom	49:Atom	50:Atom	51:Atom	52:Atom	53:Atom	
54:Atom	55:Atom	56:Atom	57:Atom	58:Atom	59:Atom	60:Atom	61:Atom	
66:CLASS	68:CLASS	69:CLASS	70:CLASS	71:CLASS	72:CLASS	73:CLASS		
74:CLASS	75:CLASS	76:CLASS	77:CLASS	78:CLASS	79:CLASS	80:CLASS		
81:CLASS	89:CLASS	90:CLASS						